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DRAFT ARCHITECTURAL COATINGS SPECIATION PROFILES AND MIR VALUES

Based on the Draft CA Emission Inventory Development and Reporting System (CEIDARS) Speciation Profiles and Nov. 2000 MIR Values [1]

SOLVENT BORNE ARCHITECTURAL COATINGS (ARB 1998 SURVEY)

WEIGHT % of TOG [2]	CUMULATIVE WT %	CAS	CHEMICAL NAME (Top 10)	MIR VALUES	UNCERTAINTY RANKING
71	71	8704	DISTILLATES/NAPHTHA/MINERAL SPIRITS	0.51 - 8.07	[see footnote 3]
5	75	1330207	ISOMERS OF XYLENE {C8 DISUBSTITUTED BENZENES}	7.48	3
3	79	108883	TOLUENE	3.97	2c
2	81	78933	METHYL ETHYL KETONE {MEK} {2-BUTANONE}	1.48	1
2	83	64175	ETHYL ALCOHOL	1.69	1
2	85	123864	N-BUTYL ACETATE	0.89	2
2	87	9996	AGGREGATED VOCS < 1.0%	-	-
2	88	71556	1,1,1-TRICHLOROETHANE	0.00	6d
1	89	75092	DICHLOROMETHANE {METHYLENE CHLORIDE}	0.07	6d
1	90	67630	ISOPROPYL ALCOHOL	0.71	1

Footnotes:

1. For most chemicals, Maximum Incremental Reactivity (MIR) Values and uncertainty values were obtained from Dr. Carter's website (http://www.cert.ucr.edu/~carter/reactdat.htm#data), "VOC Reactivity Data (Excel-97 format) as of November 13, 2000".
For "distillates/naphtha/mineral spirits", MIR values and uncertainty values were obtained from the the document "Initial Statement of Reasons for the Proposed Amendments to the Regulation for Reducing Volatile Organic Compound Emissions from Aerosol Coating Products and Proposed Tables of Maximum Incremental Reactivity Values, and Proposed Amendments to Method 310, 'Determination of Volatile Organic Compounds in Consumer Products' ", dated May 5, 2000, prepared by the California Air Resources Board.

2. In the California emission inventory database, hydrocarbon/organic emissions are stored in the database in terms of Total Organic Gas (TOG), not VOC. Normally, VOC emissions are calculated by multiplying TOG by the Fraction Reactive Organic Gas (FROG). (The FROG is the percentage of the speciation profile that is defined as photochemically reactive). However, for architectural coatings, the reported VOC emissions from the 1998 Architectural Coatings Survey were used in the emission inventory to ensure consistency with the survey data. The TOG value was then derived (back-calculated), using the VOC data from the survey and the FROG.

3. For "distillates/naphtha/mineral spirits", the designated uncertainty factor is 1.15.
For other chemicals, see the attached uncertainty rankings for descriptions of the uncertainty codes.

Items shown in brackets are chemical synonyms.

DRAFT ARCHITECTURAL COATINGS SPECIATION PROFILES AND MIR VALUES

Based on the Draft CA Emission Inventory Development and Reporting System (CEIDARS) Speciation Profiles and Nov. 2000 MIR Values [1]

WATER BORNE ARCHITECTURAL COATINGS (ARB 1998 SURVEY)

WEIGHT % of TOG [2]	CUMULATIVE WT %	CAS	CHEMICAL NAME (Top 10)	MIR VALUES	UNCERTAINTY RANKING
27	27	25265774	2,2,4-TRIMETHYL-1,3-PENTANEDIOL ISOBUTYRATE {TEXANOL}	0.89	3
27	54	57556	PROPYLENE GLYCOL	2.75	1
15	69	107211	ETHYLENE GLYCOL	3.36	2
9	78	9996	AGGREGATED VOCS < 1.0%	-	-
5	83	8704	DISTILLATES/NAPHTHA/MINERAL SPIRITS	0.51 - 8.07	[see footnote 3]
4	87	112345	2-(2-BUTOXYETHOXY)ETHANOL {BUTYL CARBITOL}	2.70	3
4	91	108054	VINYL ACETATE	3.28	5
3	94	67561	METHYL ALCOHOL {METHANOL}	0.71	1
1	94	111773	METHYL CARBITOL {2-(2-METHOXYETHOXY)ETHANOL} {DEGME}	2.90	3
1	95	111762	BUTYL CELLOSOLVE {2-BUTOXYETHANOL} {EGBE}	2.90	1

Footnotes:

1. For most chemicals, Maximum Incremental Reactivity (MIR) Values and uncertainty values were obtained from Dr. Carter's website (http://www.cert.ucr.edu/~carter/reactdat.htm#data), "VOC Reactivity Data (Excel-97 format) as of November 13, 2000".
For "distillates/naphtha/mineral spirits", MIR values and uncertainty values were obtained from the the document "Initial Statement of Reasons for the Proposed Amendments to the Regulation for Reducing Volatile Organic Compound Emissions from Aerosol Coating Products and Proposed Tables of Maximum Incremental Reactivity Values, and Proposed Amendments to Method 310, 'Determination of Volatile Organic Compounds in Consumer Products' ", dated May 5, 2000, prepared by the California Air Resources Board.

2. In the California emission inventory database, hydrocarbon/organic emissions are stored in the database in terms of Total Organic Gas (TOG), not VOC. Normally, VOC emissions are calculated by multiplying TOG by the Fraction Reactive Organic Gas (FROG). (The FROG is the percentage of the speciation profile that is defined as photochemically reactive). However, for architectural coatings, the reported VOC emissions from the 1998 Architectural Coatings Survey were used in the emission inventory to ensure consistency with the survey data. The TOG value was then derived (back-calculated), using the VOC data from the survey and the FROG.

3. For "distillates/naphtha/mineral spirits", the designated uncertainty factor is 1.15.
For other chemicals, see the attached uncertainty rankings for descriptions of the uncertainty codes.

Items shown in brackets are chemical synonyms.

Uncertainty Rankings and Descriptions

Uncertainty Ranking	Description
1	Considered to be relatively certain, or some uncertainties but reactivity is not expected to change significantly.
2	Uncertain mechanism may change somewhat if refined, but change is expected to be less than a factor of two. If the compound is predicted to inhibit O3, changes are not expected to affect predicted inhibition. This code is also used for compounds whose reactivities are expected to be highly sensitive to ambient conditions or to changes in the base mechanism.
3	Uncertain and may change if compound is studied (or studied further) or estimation methods are updated. Change in MIR could be as much as a factor of two. This code is also used for (1) compounds whose reactivities are expected to be sensitive to the representation of the reactive products, whose accuracy is difficult to test experimentally and (2) compounds whose reactivities are expected to be highly sensitive to ambient conditions or to changes in the base mechanism.
4	Uncertain and is expected to change if compound is studied or estimation methods are updated. It is recommended that uncertainty adjustments be employed in regulatory applications.
5	Non-negligible chance of the estimate being incorrect in significant respects. It is recommended that uncertainty adjustments be employed in regulatory applications.
6	Current mechanism is probably incorrect, but biases in atmospheric reactivity predictions are uncertain. It is recommended that uncertainty adjustments be employed in regulatory applications.
A	The reactivity of this compound is expected to be sensitive to ambient conditions and/or changes in the base mechanism.
B	Some uncertainty due to differences in reactivities of compounds represented by this class. Look at differences among compounds in this class for the magnitude of this uncertainty.
C	Parameterized mechanism used, with uncertain portions adjusted to fit chamber data for representative compounds.
D	Highly simplified "Placeholder" mechanism used to represent the approximate range of reactivity of this compound. Mechanism does not represent an estimate of the actual mechanism of the compound.
E	The current version of this mechanism does not represent these compounds, but based on previous studies they are expected to be O3 inhibitors under all conditions.